

Data Path : Z:\HPCHEM1\BNA F\DATA\BF072017\
 Data File : BF096919.D
 Acq On : 20 Jul 2017 21:33
 Operator : SJ/JU
 Sample : I4312-17
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 156

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON Filtering: 5
 Sampling : 1 Min Area: 3 % of largest Peak
 Start Thrs: 0.2 Max Peaks: 100
 Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.804	137	139	151	rBV	67546	137462	4.38%	0.622%
2	4.745	464	469	482	rBV	245539	391197	12.46%	1.771%
3	5.181	538	543	546	rBV	2818661	3140261	100.00%	14.220%
4	6.228	715	721	724	rBV	2457239	2779183	88.50%	12.585%
5	6.345	736	741	744	rBV	2765170	2700755	86.00%	12.230%
6	6.569	775	779	791	rBV	663443	556689	17.73%	2.521%
7	6.728	801	806	809	rBV	2170559	1941259	61.82%	8.791%
8	7.133	870	875	878	rBV	1612057	1730855	55.12%	7.838%
9	7.263	892	897	908	rVB	50647	61037	1.94%	0.276%
10	7.769	980	983	990	rBV	33135	33945	1.08%	0.154%
11	7.851	993	997	1000	rBV	943436	808319	25.74%	3.660%
12	8.927	1175	1180	1184	rBV	2308588	2377667	75.72%	10.767%
13	9.327	1244	1248	1251	rBV	408493	368731	11.74%	1.670%
14	9.598	1289	1294	1298	rBV	833658	705924	22.48%	3.197%
15	10.386	1423	1428	1431	rBV	1339333	1261091	40.16%	5.711%
16	10.521	1448	1451	1453	rBV	39566	40784	1.30%	0.185%
17	10.969	1521	1527	1529	rBV2	33423	32367	1.03%	0.147%
18	11.074	1541	1545	1548	rBV	613704	540468	17.21%	2.447%
19	12.663	1810	1815	1818	rBV	1444221	1400768	44.61%	6.343%
20	13.568	1964	1969	1974	rBV	84659	97336	3.10%	0.441%
21	13.698	1987	1991	1995	rBV	531436	478240	15.23%	2.166%
22	15.068	2219	2224	2229	rBV	444010	498479	15.87%	2.257%

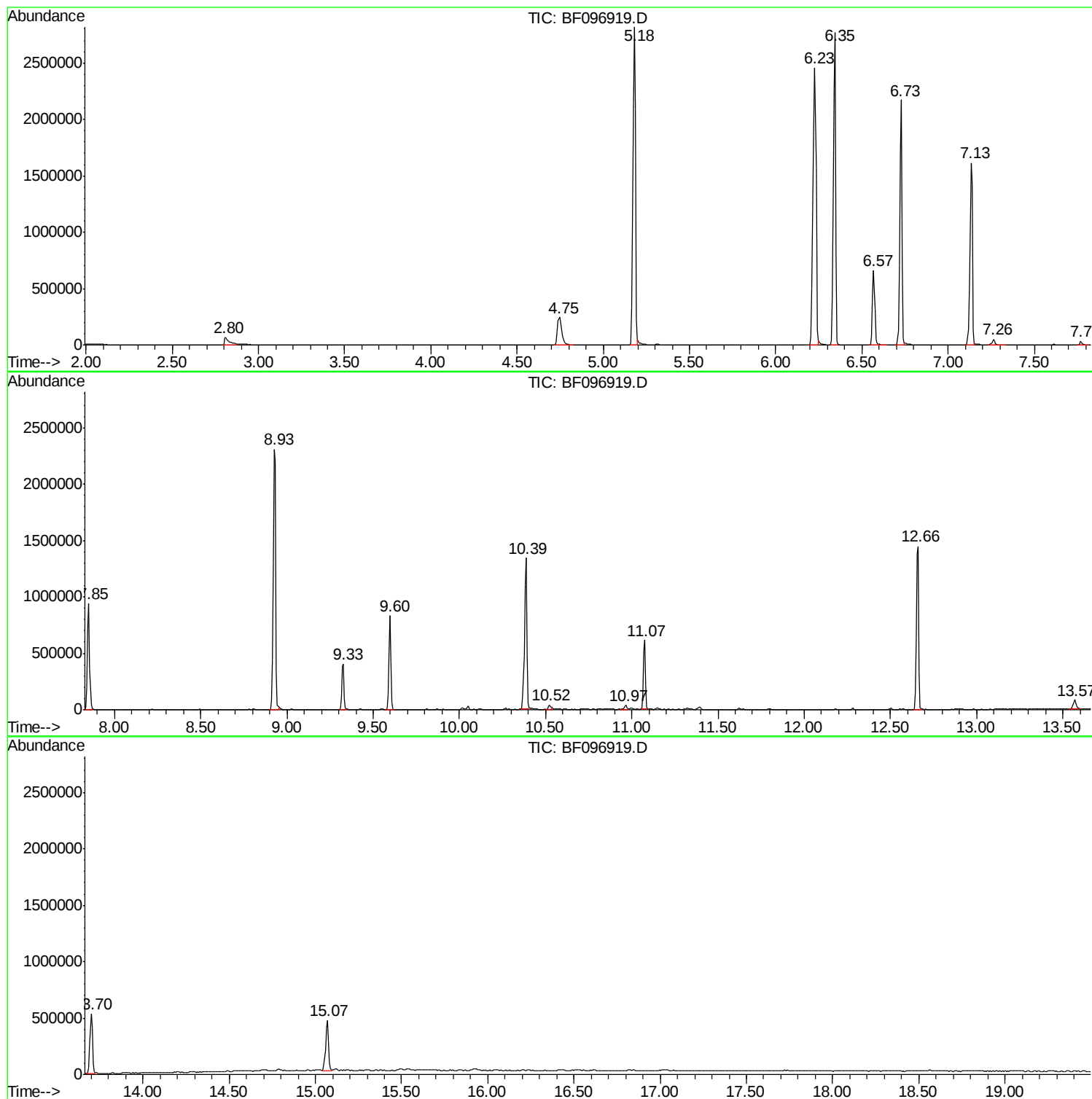
Sum of corrected areas: 22082817

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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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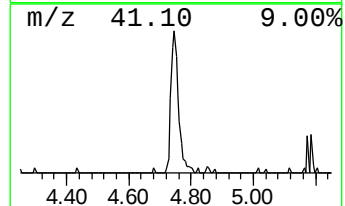
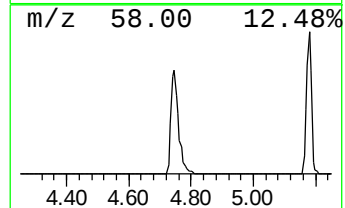
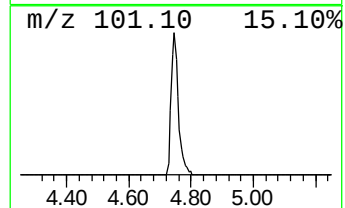
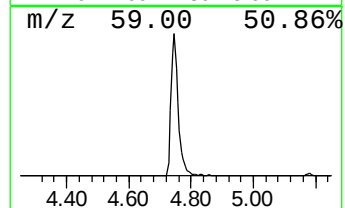
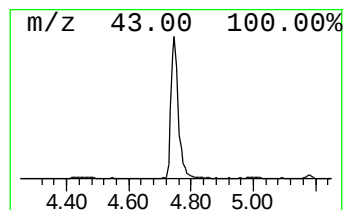
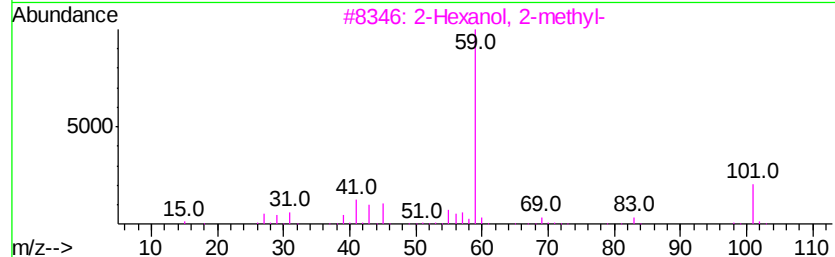
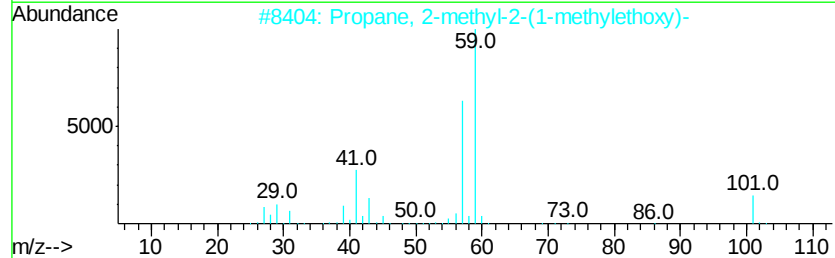
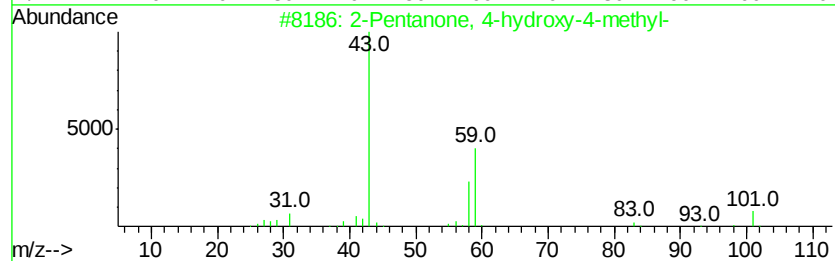
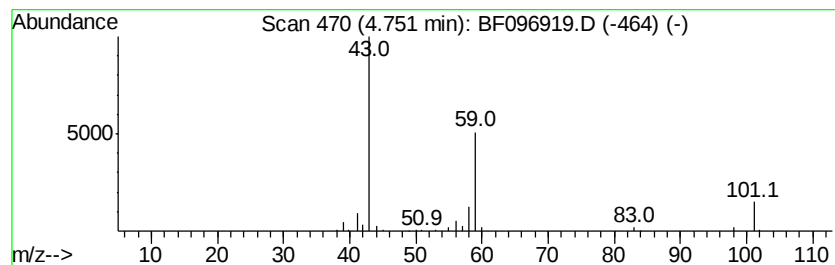
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.75	14.05 ng	391197	1,4-Dichlorobenzene-d4	6.57

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42
3		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4		3-Hexanol	102	C6H14O	000623-37-0	33
5		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33



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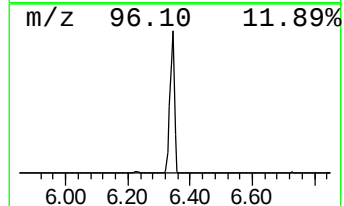
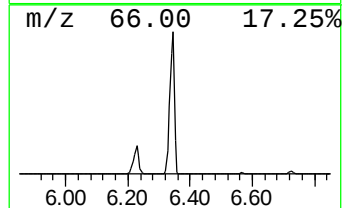
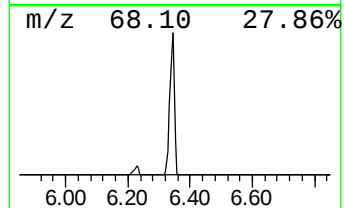
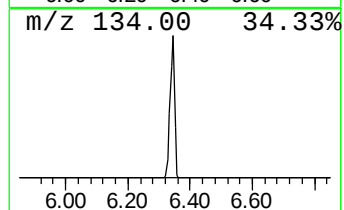
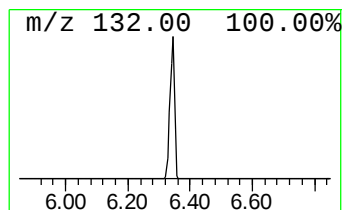
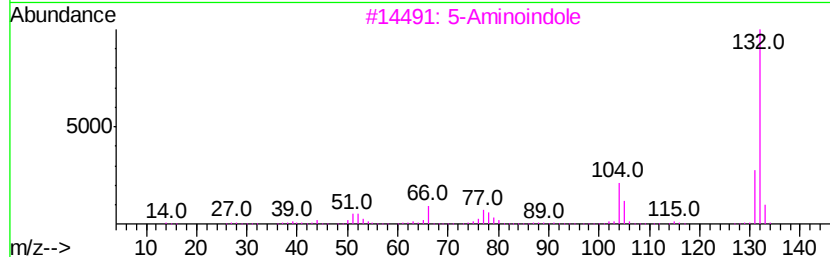
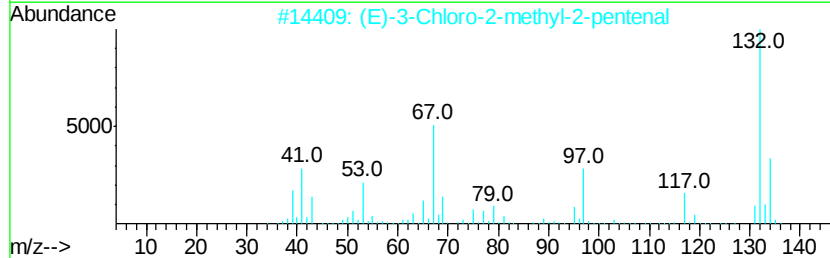
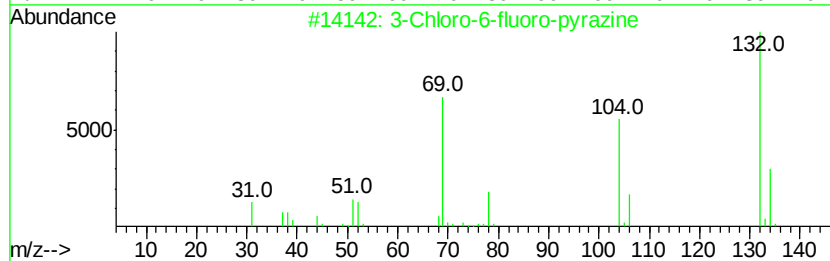
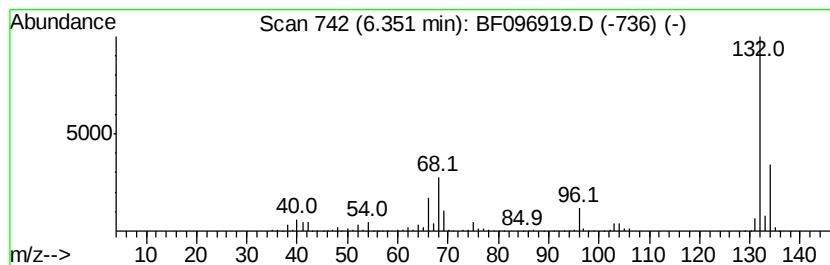
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Peak Number 3 unknown6.35 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.35	97.03 ng	2700760	1,4-Dichlorobenzene-d4	6.57

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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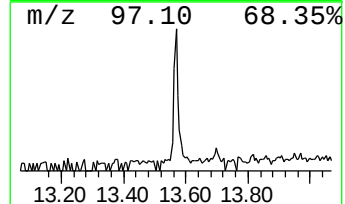
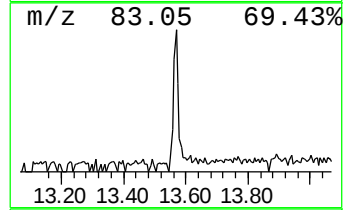
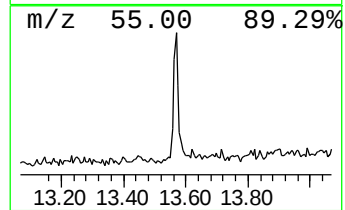
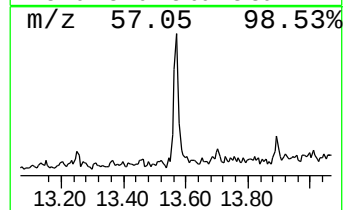
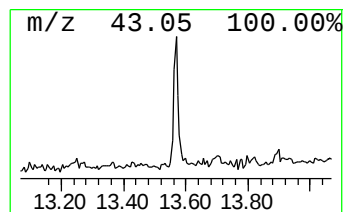
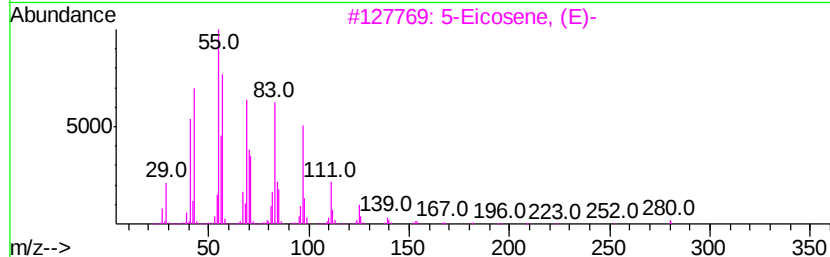
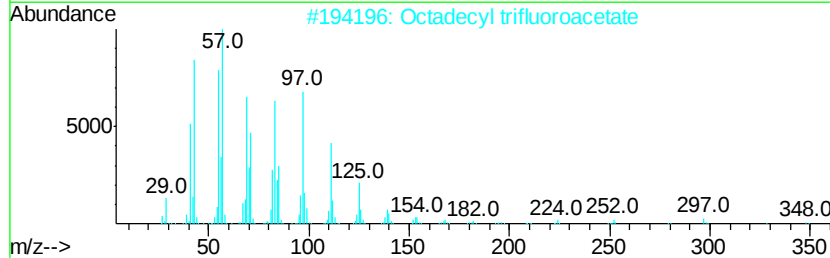
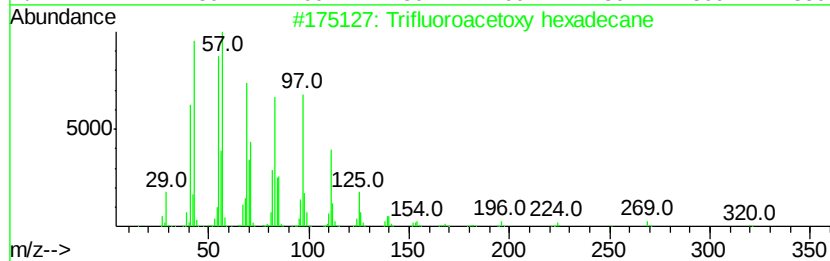
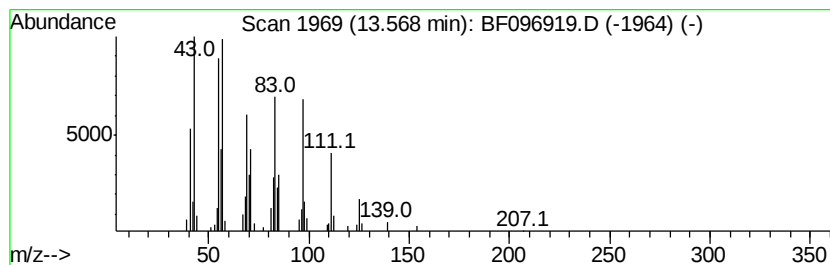
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Peak Number 5 Trifluoroacetoxy hexadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.57	4.07 ng	97336	Chrysene-d12	13.70

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
2		Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	91
3		5-Eicosene, (E)-	280	C20H40	074685-30-6	91
4		Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	90
5		Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	90



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.75	14.1	ng	391197	1	6.57	556689	20.0
unknown6.35	6.35	97.0	ng	2700760	1	6.57	556689	20.0
Trifluoroacetoxy ...	13.57	4.1	ng	97336	5	13.70	478240	20.0